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Coronoid systems with perfect matchings

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Abstract

A hexagonal system is a finite 2-connected plane graph in which every interior face is bounded by a regular hexagon. A coronoid system is obtained from a hexagonal system by deleting some interior vertices and/or interior edges such that a unique interior face which is bounded by a polygon with more than six edges emerges, and each edge on the outer perimeter belongs to a hexagon. In this paper, a necessary and sufficient condition is given for a coronoid system to have perfect matchings. Moreover, a criterion is established for those coronoid systems with perfect matchings that possess some edges which do not belong to any perfect matching.

1. Introduction

A hexagonal system (HS) [12], also called benzenoid system [5], honeycomb system and hexagonal animal [7], is a finite 2-connected plane graph in which every interior face is bounded by a regular hexagon. Hence all the hexagons of a HS H are congruent. A coronoid system (CS) G is obtained from a HS H by deleting some interior vertices and/or some interior edges such that a unique interior face bounded by a polygon with more than six edges emerges, and each edge on the outer perimeter belongs to a hexagon. The graph shown in Fig. 1(a) is a CS, the corresponding HS from which it is obtained is depicted in Fig. 1(b). Fig. 1(c) shows a graph which is not a CS since it has five edges on the outer perimeter not belonging to any of its hexagon.

A polyhex graph is either a HS or a CS [2]. A perfect matching of a graph G is an independent edge set of G such that every vertex of G is incident with an edge in the set. A perfect matching of a polyhex graph is also called a Kekulé structure by chemists [2, 5]. As pointed out by chemists [3], it is of chemical relevance to decide whether or not a given polyhex graph has a perfect matching since a polyhex graph is the skeleton of a benzenoid hydrocarbon molecule or a coronoid hydrocarbon molecule if and only if it has a perfect matching. Since a polyhex graph is a bipartite graph, criteria for the existence of perfect matchings in bipartite graphs (cf. [6, 9]) can be used to decide whether or not a given polyhex graph has a perfect matching.

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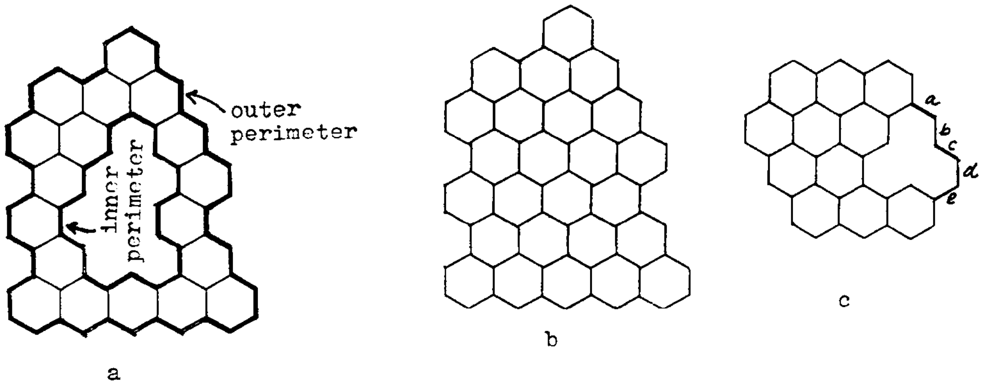

Fig. 1.

Taking into account the speciality of polyhex graphs, it is natural to find better criteria for polyhex graphs which do not apply to general bipartite graphs not being polyhex graphs. In fact, the existence of perfect matchings in a HS has been intensively studied and many results have been reported [4, 10, 12, 14, 15]. But all the known results were restricted to HSs, not any criterion for a CS to have perfect matchings has been reported. In this paper we will fill this gap. We give a necessary and sufficient condition for a CS to have perfect matchings.

Among the polyhex graphs with perfect matchings it may happen that some edges of a polyhex graph belong to all the perfect matchings of the polyhex graph, or do not belong to any perfect matching of the polyhex graph. These edges are said to be fixed double bonds and fixed single bonds, respectively [1]. A fixed bond is either a fixed double bond or a fixed single bond. A polyhex graph with perfect matchings is said to be essentially disconnected (ED) if it possesses some fixed bonds. The existence of ED polyhex graphs has proved to be very useful in certain enumeration techniques of perfect matchings [3]. Many criteria have been given to recognize ED HSs [1, 8, 11, 13]. Only one necessary and sufficient condition for a CS to be ED is reported in [16]. But this criterion does not shed any light on how to find fixed bonds in a ED CS. In this paper we give a structural characterization which amounts to be a necessary and sufficient condition for a CS to be ED.

2. A necessary and sufficient condition for a CS to have perfect matchings

In the following we use $C(\mathrm{o})$ and $C(\mathrm{i})$ to denote the outer perimeter and the inner perimeter of a CS G.

Definition 2.1. A straight line segment P_1P_2 is called an elementary cut segment of a CS G if:

(1) each of P_1 and P_2 is the centre of an edge lying on $C(\mathrm{o})$ or $C(\mathrm{i})$;

(2) P_1P_2 is orthogonal to one of the three edge directions;

(3) any point of P_1P_2 is either an interior or a boundary point of some hexagon of G.

The set of all edges intersected by an elementary cut segment P_1P_2 is called an elementary cut realized by P_1P_2.

Definition 2.2. A broken line segment $P_1P_2P_3$ is called a generalized cut segment of a CS G if

(1) each of P_1 and P_3 is the centre of an edge lying on $C(\mathrm{o})$ or $C(\mathrm{i})$, and P_2 is the centre of a hexagon of G:

(2) P_1P_2 is orthogonal to one of the three edge directions, P_1P_2 and P_2P_3 form an angle of $\pi/3$;

(3) any point of $P_1P_2P_3$ is either an interior or a boundary point of some hexagon of G.

The set of all edges intersected by a generalized cut segment $P_1P_2P_3$ is called a generalized cut realized by $P_1P_2P_3$.

Definition 2.3. A special edge cut (SE-cut) is either an elementary cut realized by an elementary cut segment or a generalized cut realized by a generalized cut segment.

By the above definitions it is easy to see that for a CS G each SE-cut C has exactly two edges on $C(\mathrm{o})$ or $C(\mathrm{i})$. If these two edges are simultaneously on $C(\mathrm{o})$ or $C(\mathrm{i})$, C is said to be a SE-cut of type I, otherwise C is said to be a SE-cut of type II. For example, for the CS G depicted in Fig. 2 the SE-cut realized by P_1P_2 is of type I, while the other SE-cuts, realized by $P_{1a}P_{2a}$, or by $P_{1b}P_{2b}$, or by $P_{1c}P_{2c}P_{3c}$ are of type II.

In the following we make the convention that the vertices of a CS G in question have been coloured black and white such that the end vertices of any edge have different colours. Let C be a SE-cut of G. By $G - C$ we denote the subgraph obtained from G by deleting all the edges of C. Evidently, $G - C$ is connected if C is of type II; and $G - C$ has two components if C is of type I. Let C_1, C_2 be two disjoint SE-cuts of type II. Then $G - C_1 - C_2$ has two components (cf. Fig. 2).

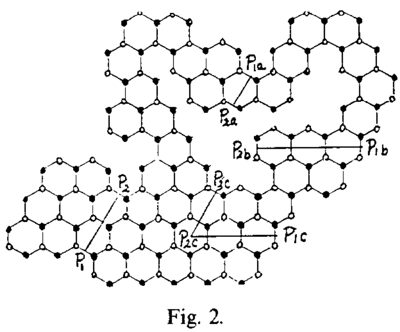

Fig. 2.

Definition 2.4. Let C_1 and C_2 be two disjoint SE-cuts of type II, $\{C_1, C_2\}$ is said to be a standard combination of type II if the end vertices of the edges of C_1 and C_2 have the same colour when they lie in the same component of $G - C_1 - C_2$.

In Fig. 2 let C_1 be the SE-cut realized by $P_{1a}P_{2a}$, C_2 be the SE-cut realized by $P_{1b}P_{2b}$, and C_3 be the SE-cut realized by $P_{1c}P_{2c}P_{3c}$. Then $\{C_1, C_2\}$ and $\{C_1, C_3\}$ are standard combinations of type II, while $\{C_2, C_3\}$ is not a standard combination.

For any set S of vertices in G, we define the neighbour set of S in G to be the set of all vertices adjacent to vertices in S; and this set is denoted by $N(S)$. For a graph H in which vertices are coloured black and white, denote by $B(H)$ and $W(H)$ the set of black vertices and the set of white vertices, respectively. For a set S of vertices in G, the subgraph of G whose vertex set is S and whose edge set is the set of those edges of G that have both ends in S is called the subgraph of G induced by S, and is denoted by $\langle S \rangle$.

Let C be a SE-cut of type I, $\{C_1, C_2\}$ be a standard combination of type II. Denote by G_1 and G_2 the two components of $G - C$ or $G - C_1 - C_2$. It is not difficult to see that G_1 and G_2 can be expressed as: $G_1 = \langle X_1 \cup N(X_1) \rangle$, $G_2 = \langle X_2 \cup N(X_2) \rangle$, where $X_1 \cup N(X_2) = W(G)$ and $X_2 \cup N(X_1) = B(G)$, or $X_1 \cup N(X_2) = B(G)$ and $X_2 \cup N(X_1) = W(G)$. Let us put $D(G_i) = |N(X_i)| - |X_i|$ for $i = 1, 2$. Evidently, for a CS G with $|B(G)| = |W(G)|$, we have $D(G_1) = D(G_2)$. In this case, we put $D(C) = D(G_1) = D(G_2)$, or $D(C_1, C_2) = D(G_1) = D(G_2)$.

The following theorem due to Hall [6] is useful in the proof of our main theorem.

Theorem 2.5. *Let G be a bipartite graph with bipartition (X, Y). Then G has a matching that saturates every vertex in X if and only if $|N(S)| \geqslant |S|$ for all $S \subset X$, where $N(S)$ is the neighbour set of S in G.*

We are now in the position to give our main result.

Theorem 2.6. *Let G be a CS. Then G has a perfect matching if and only if:*

(1) $|W(G)| = |B(G)|$,

(2) $D(C) \geqslant 0$ *for every SE-cut C of type* I: *and* $D(C_1, C_2) \geqslant 0$ *for every standard combination* $\{C_1, C_2\}$ *of type* II.

Proof. *Necessity*: Suppose that G has a perfect matching. Since G is bipartite, condition (1) holds. Let G_1 be one of the two components of $G - C$, where C is a SE-cut of type I. Let us put $G_1 = \langle X_1 \cup N(X_1) \rangle$. Since G is a bipartite graph with bipartition $(W(G), B(G))$, and $X_1 \subset W(G)$ or $X_1 \subset B(G)$, by Theorem 2.5 $|N(X_1)| \geqslant |X_1|$. Hence $D(G) = D(G_1) = |N(X_1)| - |X_1| \geqslant 0$. The same is true for $D(C_1, C_2)$, according to the same reasoning, when $\{C_1, C_2\}$ is a standard combination of type II.

Sufficiency: It suffices to prove that if G has no perfect matching and condition (1) holds, then there exists a SE-cut C of type I satisfying $D(C) < 0$, or a standard combination $\{C_1, C_2\}$ of type II satisfying $D(C_1, C_2) < 0$.

Since G has no perfect matching, by Theorem 2.5 there exists a subset $S \subset B(G)$ or $\subset W(G)$ such that $|S| > |N(S)|$. Let $G' = \langle S \cup N(S) \rangle$. Denote by $\overline{G'} = G - G'$ the subgraph of G obtained by deleting all the vertices of G' together with their incident edges. We claim that there is an $S \subset B(G)$ or $\subset W(G)$ satisfying $|S| > |N(S)|$ such that both G' and $\overline{G'}$ are connected. Suppose that G' is not connected and has t components $G'_1, \ldots, G'_t$ $(t \geqslant 2)$. Then we have $G'_i = \langle S_i \cup N(S_i) \rangle$, $i = 1, \ldots, t$; where $S = S_1 \cup S_2 \cup \cdots \cup S_t$, $S_i \cap S_j = \emptyset$ for $i \neq j$; and $N(S) = N(S_1) \cup N(S_2) \cup \cdots \cup N(S_t)$, $N(S_i) \cap N(S_j) = \emptyset$ for $i \neq j$. Since $|S| > |N(S)|$, there is at least one set S_i $(1 \leqslant i \leqslant t)$ such that $|S_i| > |N(S_i)|$. We replace S by S_i and ensure that the induced subgraph $\langle S_i \cup N(S_i) \rangle$ is connected. Now, without loss of generality, we may assume that G' is connected. If $\overline{G'}$ is also connected, there is nothing to prove. If $\overline{G'}$ is not connected, $\overline{G'}$ has h $(\geqslant 2)$ components $\overline{G'_1}, \ldots, \overline{G'_h}$. We can put $\overline{G'} = \langle T \cup N(T) \rangle$, $\overline{G'_j} = \langle T_j \cup N(T_j) \rangle$, $j = 1, \ldots, h$, where $T = T_1 \cup \cdots \cup T_h$, $N(T) = N(T_1) \cup \cdots \cup N(T_h)$, $T_i \cap T_j = \emptyset$ and $N(T_i) \cap N(T_j) = \emptyset$ for $i \neq j$. By our assumption condition (1) holds, hence $|S| + |N(T)| = |N(S)| + |T|$. Since $|S| > |N(S)|$, we have $|T| > |N(T)|$, i.e. $\sum_j |T_j| > \sum_j |N(T_j)|$. Therefore, there is at least one set T_j $(1 \leqslant j \leqslant h)$ such that $|T_j| > |N(T_j)|$. It is evident that both $\langle T_j \cup N(T_j) \rangle$ and $G - \langle T_j \cup N(T_j) \rangle = G' \cup \langle T_1 \cup N(T_1) \rangle \cup \cdots \cup \langle T_{j-1} \cup N(T_{j-1}) \rangle \cup \langle T_{j+1} \cup N(T_{j+1}) \rangle \cup \cdots \cup \langle T_h \cup N(T_h) \rangle$ are connected. Then T_j is a set S which has the required properties.

We have shown that there is an $S \subset B(G)$ or $S \subset W(G)$ with $|S| > |N(S)|$ such that both $G' = \langle S \cup N(S) \rangle$ and $\overline{G'} = G - G'$ are connected. Now we prove that G' has some edges lying on $C(\mathrm{o})$ or $C(\mathrm{i})$ of G. Let $n_i(S)$, $i = 2, 3$ denote the number of vertices of S with valency i in G. Evidently, each vertex in S has the same valency in G' as in G. Let $E(G')$ be the edge set of G'. Then we have $3n_3(S) + 2n_2(S) = |E(G')| \leqslant 3|N(S)| < 3|S| = 3(n_2(S) + n_3(S))$. Hence $n_2(S) > 0$. This implies that S has some vertices of valency 2 in G. These vertices must lie together with their incident edges on $C(\mathrm{o})$ or $C(\mathrm{i})$ of G. Therefore, G' has some edges lying on $C(\mathrm{o})$ or $C(\mathrm{i})$ of G. According to the same reasoning, $\overline{G'}$ also has some edges lying on $C(\mathrm{o})$ or $C(\mathrm{i})$ of G.

Denote by $(G', \overline{G'})$ the set of edges of G in which each edge has one end vertex in G' and the other end vertex in $\overline{G'}$. Then $(G', \overline{G'})$ is an edge cut of G, and the end vertices of the edges in $(G', \overline{G'})$ have the same colour when they belong to the same component of $G - (G', \overline{G'})$, i.e. G' or $\overline{G'}$. Suppose that J is a Jordan curve in the plane separating G' from $\overline{G'}$. Then J must intersect all the edges in $(G', \overline{G'})$. Let J intersect each edge in $(G', \overline{G'})$ at the midpoint of the edge, and turn at the centre of a hexagon of G. Since the end vertices of the edges in $(G', \overline{G'})$ have the same colour when they lie in the same component G' or $\overline{G'}$, at each turning point of J the angle must be 60° or 300°. If $(G', \overline{G'})$ does not contain any edge on $C(\mathrm{o})$ or $C(\mathrm{i})$ of G, J does not traverse $C(\mathrm{o})$ or $C(\mathrm{i})$ of G. Hence $C(\mathrm{o})$ is contained in G' and $C(\mathrm{i})$ is contained in $\overline{G'}$, or vice versa since both G' and $\overline{G'}$ have some edges lying on $C(\mathrm{o})$ or $C(\mathrm{i})$ of G as mentioned above. Now we start from S, delete some vertices in S (cf. the vertices $1, 2, \ldots, n$ found within a trapezoid in the diagram depicted in Fig. 3) to get a new S^* such that the corresponding new Jordan curve J^* intersects some edges of $C(\mathrm{i})$ of G; then S^*

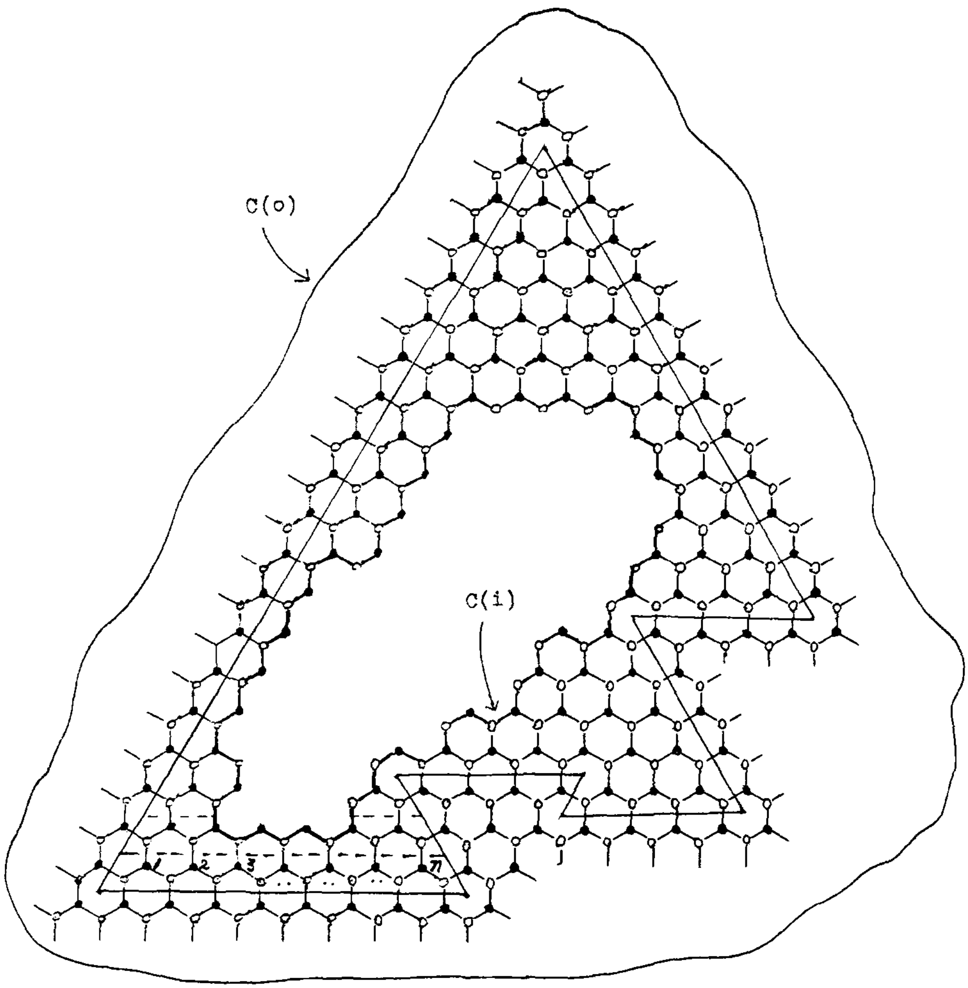

Fig. 3.

maintains the properties of S, i.e. $|S^*| > |N(S^*)|$, while both $G^{*\prime} = \langle S^* \cup N(S^*) \rangle$ and $\overline{G^{*\prime}} = G - G^{*\prime}$ are connected, and $(G^{*\prime}, \overline{G^{*\prime}})$ contains some edges on $C(\mathrm{i})$ of G.

Before continuing, we introduce some symbols:

$A = \{G' \mid G' = \langle S \cup N(S) \rangle$ such that $S \subset B(G)$ or $S \subset W(G)$, $|S| > |N(S)|$, both G' and $\overline{G'} = G - G'$ are connected, $(G', \overline{G'})$ has some edges on $C(\mathrm{o})$ or $C(\mathrm{i})\}$,

$\alpha = \min\{D(G') = |N(S)| - |S| \mid G' \in A\}$,

$A_\alpha = \{G' \mid G' \in A,\ D(G') = \alpha\}$,

$\beta = \max\{|V(G')| \mid G' \in A_\alpha\}$,

$A_\beta = \{G' \mid G' \in A_\alpha, |V(G')| = \beta\}$.

Let $G' \in A_\beta$. Any Jordan curve J in the plane which separates G' from $\overline{G'}$ must traverse at least one of the two perimeters $C(\mathrm{o})$ and $C(\mathrm{i})$ meeting each perimeter in either none or precisely two edges. Now assume that the edges in $(G', \overline{G'})$ are met by J in the cyclic order $e_1, e_2, \ldots, e_n$. Without loss of generality, we may suppose that we have one of the following two cases.

Case 1: e_1 and e_n lie simultaneously on $C(\mathrm{o})$ or $C(\mathrm{i})$ of G, and no other edge of $(G, \overline{G'})$ lies on $C(\mathrm{o})$ or $C(\mathrm{i})$ of G.

Case 2: e_1 and e_n lie on $C(\mathrm{o})$ and for some r $(2 < r < n)$, e_{r-1} and e_r lie on $C(\mathrm{i})$, and no other edge of $(G', \overline{G'})$ lies on $C(\mathrm{o})$ or $C(\mathrm{i})$ of G.

First we consider Case 1.

Subcase 1.1: e_1 and e_n lie on $C(\mathrm{o})$ of G. If $e_1, e_2, \ldots, e_n$ are parallel, then $C = \{e_1, e_2, \ldots, e_n\}$ is realized by an elementary cut segment, and is a SE-cut of type I satisfying $D(C) = D(G') = |N(S)| - |S| < 0$. Hence C is a SE-cut having the required property mentioned at the beginning of the proof of sufficiency. Now suppose that $e_1, \ldots, e_{m-1}$ and e_m $(m < n)$ are parallel, but e_{m+1} is not parallel to them. Bear in mind that the end vertices of e_i, $i = 1, \ldots, n$ have the same colour when they belong to the same component G' or $\overline{G'}$. Hence $e_{m+1} = e_1^*$ or $e_{m+1} = e_2^*$ (see Fig. 4). Without loss of generality we may assume that $e_{m+1} = e_1^*$. If $e_{m+1}, \ldots, e_{n-1}$ and e_n are parallel, then it is evident that $C = \{e_1, \ldots, e_m, e_{m+1}, \ldots, e_n\}$ is a SE-cut of type I realized by a generalized cut segment, and satisfies $D(C) = D(G') = |N(S)| - |S| < 0$. Now suppose that $e_{m+1}, \ldots, e_{m+t-1}$ and e_{m+t} are parallel, but e_{m+t+1} is not parallel to them. We need to consider two possibilities.

Subcase 1.1.1: $e_{m+t+1} = e_3^*$ (see Fig. 4).

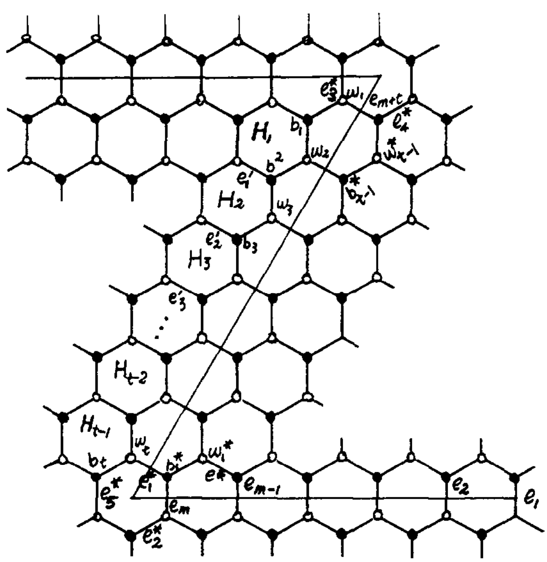

Fig. 4.

If edge $b_1w_1 \in G'$, then edge $b_1^*w_1^* \in \overline{G'}$ (see Fig. 4). Let $S^* = S \cup \{b_1^*\}$, then $N(S^*) = N(S) \cup \{w_1^*\}$. Let $G'' = \langle S^* \cup N(S^*) \rangle$. If $\overline{G''} = G - G''$ is connected, $G'' \in A$. Furthermore, $G'' \in A_\alpha$ since $D(G'') = D(G') = \alpha$. But $|V(G'')| = |V(G')| + 2 = \beta + 2 > \beta$, contradicting the selection of β. Therefore, $\overline{G''}$ is disconnected. This implies that w_1^* is on C(o) or C(i) of G. Since e_1 and e_n are on C(o) of G by our assumption, C(i) must entirely belong to G' or $\overline{G'}$. If w_1^* is on C(i), $\overline{G''} = G - G'' = G' - \{b_1^*, w_1^*\}$ will not be disconnected. Hence w_1^* is on C(o) of G. Let the component of $\overline{G''}$ connected to $e_1, \dots, e_{m-1}$ be $\overline{G_1''} = \langle T_1 \cup N(T_1) \rangle$. We claim that $|T_1| > |N(T_1)|$. Otherwise, let $S^{**} = S \cup N(T_1) \cup \{b_1^*\}$ (cf. Fig. 4). Then $N(S^{**}) = N(S) \cup T_1 \cup \{w_1^*\}$. Let $G'^* = \langle S^{**} \cup N(S^{**}) \rangle$. It is not difficult to see that $G'^* \in A$. But $D(G'^*) = D(G') + (|T_1| - |N(T_1)|)$. If $|T_1| < |N(T_1)|$, then $D(G'^*) < D(G')$, contradicting $D(G') = \alpha$. Hence $|T_1| = |N(T_1)|$. This implies that $D(G'^*) = D(G') = \alpha$. Therefore, $G'^* \in A_\alpha$. But $|V(G'^*)| > |V(G')| = \beta$, again a contradiction. Consequently, we have $|T_1| > |N(T_1)|$. Now let $C = \{e_1, \dots, e_{m-1}, e^*\}$ (see Fig. 4). C is a SE-cut of type I realized by a generalized cut segment and has the required property that $D(C) < 0$ (note that $D(C) = D(\overline{G_1''}) = |N(T_1)| - |T_1|$).

If edge $b_1w_1 \in \overline{G'}$, analogous reasoning as above shows that $\{b_1, w_1\}$ is a vertex cut of $\overline{G'}$, and b_t is on C(o) of G. We consider the following two subcases.

Subcase 1.1.1.1: e_5^* is on C(o) or C(i) of G (see Fig. 4).

First, we suppose that e_5^* is on C(o) of G. $C = \{e_1, \dots, e_m, e_5^*\}$ is a SE-cut of type I realized by an elementary cut segment. Let the two components of $G - C$ be G^* and $\overline{G^*}$, where G^* is entirely contained in G'. Put $G^* = \langle S^* \cup N(S^*) \rangle$. If $|S^*| > |N(S^*)|$, then $D(C) = D(G^*) = |N(S^*)| - |S^*| < 0$. C is thus a SE-cut of type I having the required property. If $|S^*| < |N(S^*)|$, let $S^{**} = S \cup N(S^*)$. Then $N(S^{**}) = N(S) \cup S^* \cup \{b_t\}$. Let $G^{**} = \langle S^{**} \cup N(S^{**}) \rangle$. $D(G^{**}) = |N(S^{**})| - |S^{**}| = |N(S)| - |S| - (|N(S^*)| - |S^*|) + 1 \leqslant \alpha$. By the minimality of α, we have $D(G^{**}) = \alpha$. Hence $G^{**} \in A_\alpha$. But $|V(G^{**})| > |V(G')|$, contradicting the maximality of β. Consequently, $|S^*| = |N(S^*)|$. If all the edges b_iw_i, $i = 2, \dots, t$, are on C(o) of G, let $S^{***} = S \cup N(S^*) \cup \{w_1, \dots, w_t\}$. Then $N(S^{***}) = N(S) \cup S^* \cup \{b_1, \dots, b_t\}$. Let $G^{***} = \langle S^{***} \cup N(S^{***}) \rangle$. Evidently, $\overline{G^{***}} = G - G^{***}$ is connected, and $D(G^{***}) = D(G') = \alpha$. Hence $G^{***} \in A_\alpha$. But $|V(G^{***})| > |V(G')| = \beta$, again a contradiction, which implies that some of the edges $b_2w_2, \dots, b_tw_t$ are not on C(o). Thus there exist $d_f \geqslant 0$ and i_f, $f = 1, \dots, p$ satisfying $1 < i_1$, $i_1 + d_1 + 1 < i_2, \dots, i_{p-1} + d_{p-1} + 1 < i_p, i_p + d_p < t$ such that hexagons $H_{i_f}, H_{i_f+1}, \dots, H_{i_f+d_f} \in G$ (see Fig. 4) for $f = 1, \dots, p$; and $H_j \notin G$ for $j \neq i_f, i_f + 1, \dots, i_f + d_f$, $f = 1, \dots, p$. Let $C_f = \{e'_{i_f-1}, e'_{i_f}, \dots, e'_{i_f+d_f}\}$ ($f = 1, \dots, p$) (see Fig. 4). Note that at most one pair $\{C_{f_1}, C_{f_2}\}$ ($1 \leqslant f_1 < f_2 \leqslant p$) of them is a standard combination of type II, and all others are SE-cuts of type I (cf. Fig. 5). Let the component of $G - C_f$ or $G - C_{f_1} - C_{f_2}$ contained in $\overline{G'}$ be G_f^* or $G_{f_1f_2}^*$. Put $G_f^* = \langle S_f \cup N(S_f) \rangle$, and $G_{f_1f_2}^* = \langle S_{f_1f_2} \cup N(S_{f_1f_2}) \rangle$. If $|S_f| \leqslant |N(S_f)|$ for all $f \neq f_1, f_2$, $1 \leqslant f \leqslant p$: and $|S_{f_1f_2}| \leqslant |N(S_{f_1f_2})|$, let $S'' = S \cup N(S^*) \cup \{\bigcup_f N(S_f)\} \cup N(S_{f_1f_2}) \cup \{w_1, w_2, \dots, w_t\}$. Then $N(S'') = N(S) \cup S^* \cup \{\bigcup_f S_f\} \cup S_{f_1f_2} \cup \{b_1, \dots, b_t\}$. Let $G'' = \langle S'' \cup N(S'') \rangle$. It is not difficult to check that $G'' \in A_\alpha$, and $|V(G'')| > |V(G')| = \beta$, again a contradiction.

This contradiction indicates that there is one set S_k ($1 \leqslant k \leqslant p$) such that $|S_k| > |N(S_k)|$, or there is a standard combination $\{C_r, C_s\}$, $1 \leqslant r < s \leqslant p$, such that $|S_{rs}| > N(S_{rs})|$. Consequently, a SE-cut of type I or a standard combination of type II satisfying condition (2) in the theorem is found (cf. Fig. 5).

Now we turn to the case when e_5^* is on C(i) of G (cf. Figs. 4 and 6). By an analogous reasoning as above we can find a SE-cut C of type I satisfying $D(C) < 0$, or a standard combination $\{C_1, C_2\}$ or type II satisfying $D(C_1, C_2) < 0$, where $C_1 = \{e_1, \ldots, e_m, e_5^*\}$.

Subcase 1.1.1.2: e_5^* is in the interior of G (see Figs. 4 and 7).

The arguments are quite similar to those of the above case; we omit the details.

Subcase 1.1.2: $e_{m+t+1} = e_4^*$ (see Figs. 4 and 8).

As mentioned above, both G' and $\overline{G'}$ belong to A. Considering the edge $b_1^* w_1^*$, we may assume w.l.o.g. that $b_1^* w_1^* \in G'$. Let $G'' = G' - \{b_1^*, \ldots, b_t^*, w_1^*, \ldots, w_{t-1}^*\}$. If G'' is connected, then $G'' \in A$. But $D(G'') = D(G') - 1 = \alpha - 1 < \alpha$, contradicting the selection of α. Hence G'' has $\geqslant 2$ components (see Fig. 8) G_i'', $i = 1, 2, \ldots, d$, where the first component G_1'' is connected to the edge e_1. Let $G_i'' = \langle S_i \cup N(S_i) \rangle$. Then we have $S = S_1 \cup \cdots \cup S_d \cup \{w_1^*, \ldots, w_{t-1}^*\}$ and $N(S) = N(S_1) \cup N(S_2) \cup \cdots \cup N(S_d) \cup \{b_1^*, \ldots, b_t^*\}$. If for $1 \leqslant i \leqslant d-1$ $|S_i| \leqslant |N(S_i)|$, then we have $D(G_d'') = |N(S_d)| - |S_d| = D(G') - 1 + \sum_{i=1}^{d-1}(|S_i| - |N(S_i)|) \leqslant D(G') - 1 < \alpha$, again contradicting the selection of α. (Note that $G_d'' \in A$.) Therefore, there is a q, $1 \leqslant q \leqslant d-1$ such that $|S_q| > |N(S_q)|$. Consequently, we can find as before a SE-cut of type I or a standard combination of type II having the required property.

Subcase 1.2: e_1 and e_n are on C(i) of G. We note that in this case C(o) of G is entirely contained in G' or $\overline{G'}$. The arguments are quite similar to those of Subcase 1.1, we omit the details. But if we bear in mind that C(o) of G is entirely contained in G' or $\overline{G'}$, the discussion may be simpler than those in Subcase 1.1. In particular, consider the subcase when $e_{m+t+1} = e_3^*$ (cf. Fig. 4). If the edge $b_1 w_1$ belongs to $\overline{G'}$, we can deduce that $\overline{G'} - \{b_1, w_1\}$ is disconnected as in Subcase 1.1.1. In Subcase 1.1 we cannot decide whether or not C(i) is contained in $\overline{G'}$, thus we need to consider whether e_5^* is on C(o) or C(i) (cf. Subcase 1.1.1.1). But in Subcase 1.2 after knowing that $\overline{G'} - \{b_1, w_1\}$ is disconnected, we can come to the further conclusion that C(o) must be entirely contained in G' (otherwise, although b_1 is on C(i), deleting from $\overline{G'}$ vertex b_1 will not disconnect $\overline{G'}$ since C(o) is entirely contained in $\overline{G'}$). Therefore, we need not consider the case when e_5^* is on C(o) (cf. Subcase 1.1.1.1).

Now we consider Case 2.

We want to show that $C_1 = \{e_1, \ldots, e_{r-1}\}$ and $C_2 = \{e_r, \ldots, e_n\}$ are both SE-cuts of type II, while $\{C_1, C_2\}$ is a standard combination of type II. If C_1 is not a SE-cut of type II, then there are two integers m and t satisfying $m + t < r - 1$ such that $e_1, \ldots, e_m$ are parallel, while e_{m+1} is not parallel to these edges; furthermore $e_{m+1}, \ldots, e_{m+t}$ are parallel, while e_{m+t+1} is not parallel to them (cf. Fig. 4). Note that $G - C_1$ is connected since C_1 is of type II. It is evident that $G - C_1 - \{b_1, w_1\}$ also is connected, and the same is true for $G - C_1 - \{b_1^*, w_1^*\}$. Hence, in a similar way as in Case 1 we will find a contradiction. Therefore, C_1 is a SE-cut of type II. By the same

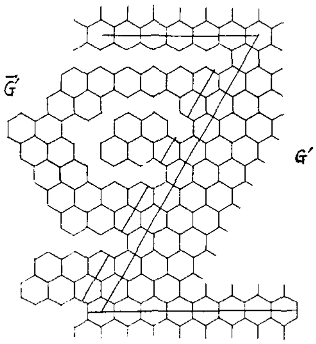

Fig. 5.

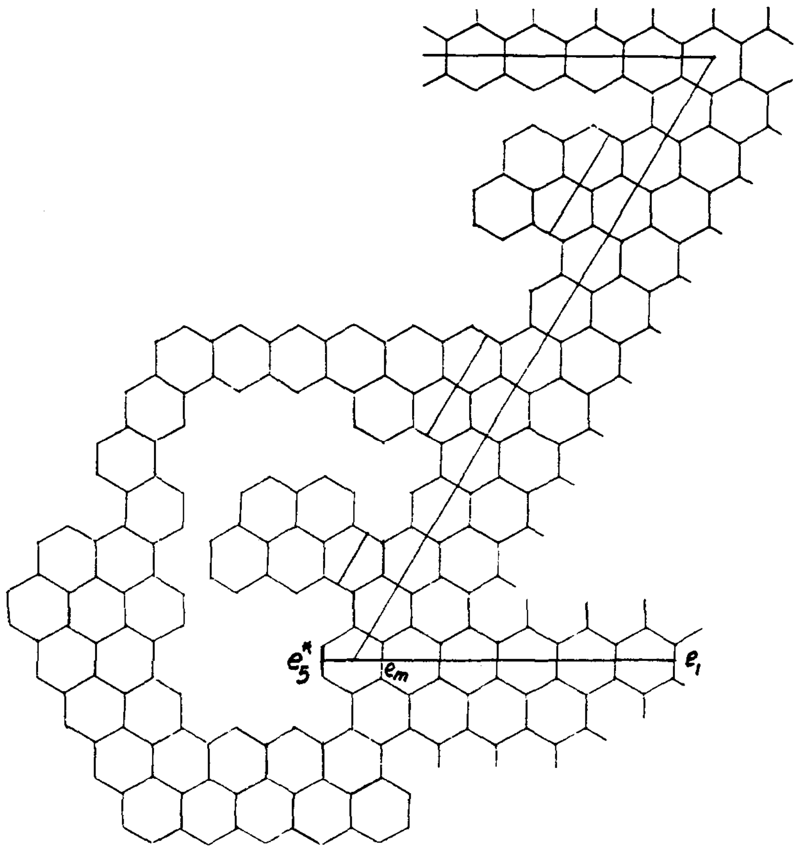

Fig. 6.

reasoning the same is true for C_2. Finally, by the definition of $(G', \overline{G'})$, $\{C_1, C_2\}$ must be a standard combination of type II.

This completes the proof of Theorem 2.6. $\square$

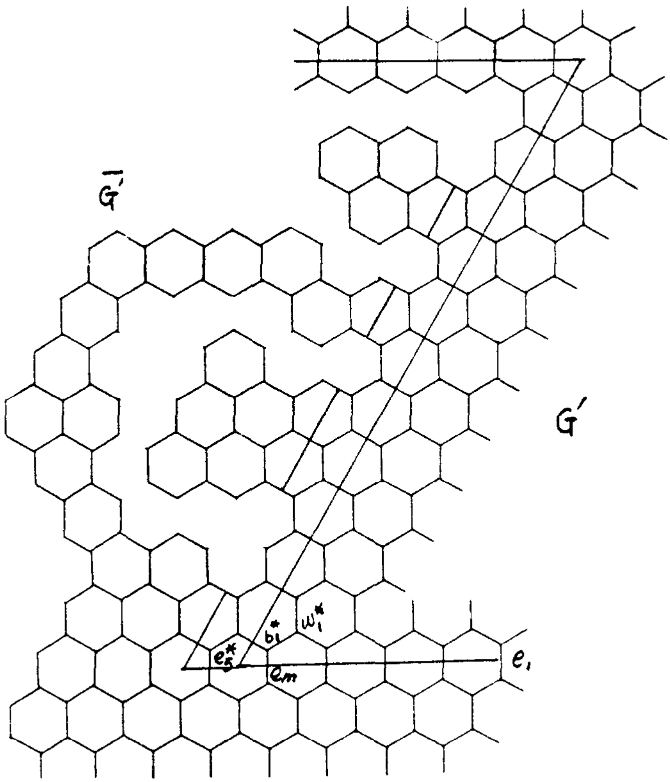

Fig. 7.

3. Essentially disconnected CSs

Now we turn our attention to ED CSs. First we introduce some more terminology.

Let G be a polyhex graph, M be a perfect matching of G. An edge e of G is said to be an M-double bond if $e \in M$, otherwise e is said to be an M-single bond. Let $E(G)$ be the edge set of G. A cycle Y of G is said to be an M-alternating cycle if the edges of Y are alternately in M and $E(G) - M$. Let N_1 and N_2 be two subsets of $E(G)$. The symmetric difference, denoted by $N_1 \oplus N_2$, is the subset of $E(G)$ consisting of those edges that belong to exactly one of N_1 and N_2, i.e. $N_1 \oplus N_2 = (N_1 \cup N_2) - (N_1 \cap N_2)$. For two different perfect matchings M_1 and M_2 of G, it is not difficult to see that the induced subgraph $\langle M_1 \oplus M_2 \rangle$ consists of some disjoint $M_1(M_2)$-alternating cycles.

Lemma 3.1. *An edge e of G is not a fixed bond if and only if e belongs to an M-alternating cycle for every perfect matching M of G.*

Proof. Let Y be an M-alternating cycle of G, where M is a perfect matching of G. Assume that $e \in Y$. Let $M' = M \oplus E(Y)$, where $E(Y)$ is the set of edges on Y.

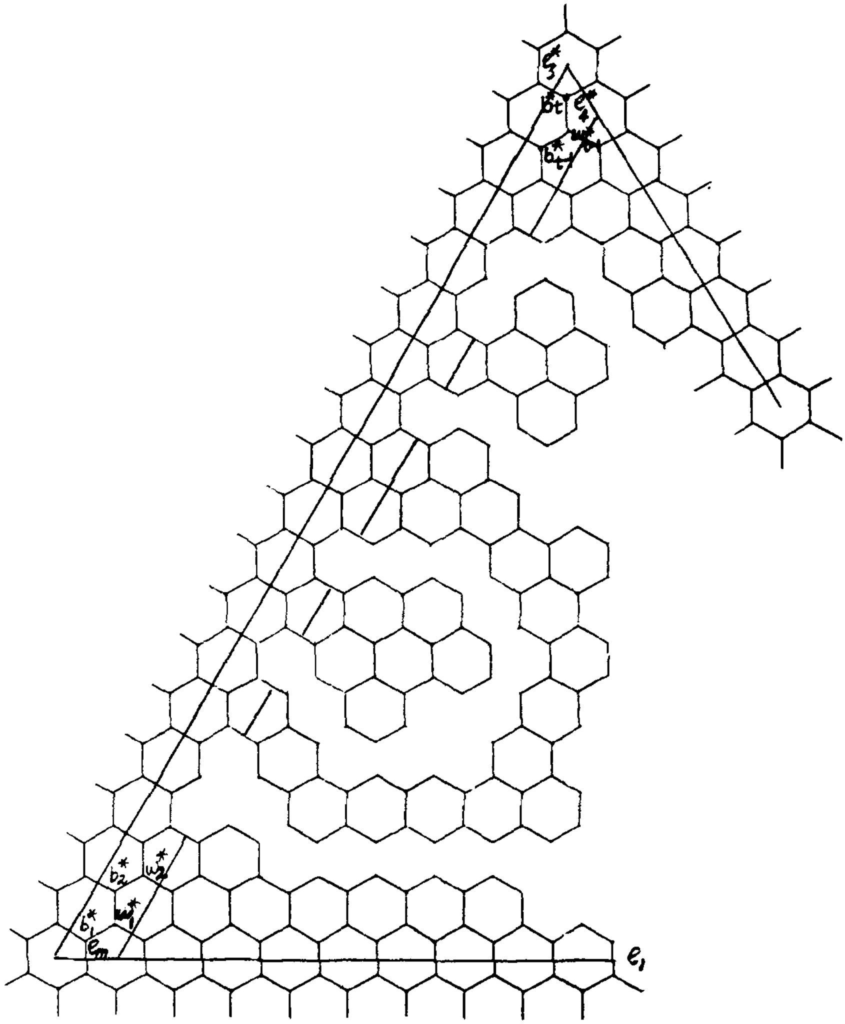

Fig. 8.

Evidently, $M' \neq M$. If e is an M-double bond, then e is an M'-single bond; and vice versa. Therefore, e is not a fixed bond.

Conversely, suppose that e is not a fixed, bond. Let M be a perfect matching of G. W.l.o.g., we assume $e \in M$. Since e is not fixed, there is a perfect matching $M' \neq M$ such that e is an M'-single bond. Then $e \in \langle M \oplus M' \rangle$, and belongs to an $M(M')$-alternating cycle. □

Lemma 3.2. *Every ED CS has some edges that are not fixed bonds.*

Proof. Let G be an ED CS. Suppose that G has h hexagons, p vertices. q edges with t edges on the perimeters. Since every hexagon has six edges, and every edge not on the perimeters belongs to two hexagons, we have $6h = t + 2(q - t)$ which together with Euler's formula $p - q + h = 0$ yields

$$p - 2h - (t/2) = 0. \tag{1}$$

Suppose that M is a perfect matching of G with r edges on the perimeters. Then M has $(p/2) - r$ edges not on the perimeters of G. If $r = t/2$, then the perimeters of G consist of two M-alternating cycles. By Lemma 3.1 all the edges on the perimeters of G are not fixed bonds. Now we assume that $r < t/2$. We want to show that there is a hexagon of G which is an M-alternating cycle. If not, each hexagon has at most two edges in the perfect matching M. Hence $2h \geqslant r + 2((p/2) - r) = p - r > p - (t/2)$ i.e. $p - 2h - (t/2) < 0$, contradicting Eq. (1) mentioned above. Therefore, there is a hexagon being an M-alternating cycle, and its six edges are not fixed bonds. □

Lemma 3.3 (Zhang and Zheng [16]). *An ED polyhex graph has some fixed single bonds on its perimeter(s).*

Lemma 3.4 (Zhang and Zheng [16]). *Let G be a polyhex graph, H be a hexagon of G. Edges e', e_1 and e'' are three consecutive edges of H. Edges $e_2, \ldots, e_n$ belong to G and satisfy:*

(1) *they are parallel to e_1,*

(2) $e_2 \in H$,

(3) *each pair of edges e_i and e_{i+1} belongs to the same hexagon of G for $i = 2, \ldots, n - 1$,*

(4) *e_n is on the perimeter of G.*

If e_1 is a fixed single bond there is a perfect matching M of G such that e' and e'' belong to M, then all the edges $e_2, \ldots, e_n$ are fixed single bonds.

Theorem 3.5 (Zhang and Zheng [16]). *A polyhex graph G has no fixed bonds if and only if each of the perimeters of G is an M-alternating cycle for some perfect matching M of G.*

We are now in the position to give our criterion which enables us to decide whether or not a CS has fixed bonds and to find some fixed single bonds (if any).

Theorem 3.6. *Let G be a CS. Then G is ED if and only if*

(1) $|w(G)| = |B(G)|$;

(2) *$D(C) \geqslant 0$ for every SE-cut of type* I, *and $D(C_1, C_2) \geqslant 0$ for every standard combination $\{C_1, C_2\}$ of type* II;

(3) *there is a SE-cut of type* I *satisfying $D(C) = 0$, or a standard combination $\{C_1, C_2\}$ satisfying $D(C_1, C_2) = 0$.*

Proof. *Sufficiency*: Conditions (1) and (2) guarantee that G has a perfect matching (Theorem 2.6). We now want to show that G has some fixed single bonds. Suppose that G has a SE-cut C of type I such that $D(C) = 0$. Let the two components of $G - C$ be G_1 and G_2. For any perfect matching M of G, since the end vertices of the edges in C have the same colour when they are in the same component G_1 or G_2, the number of M-double bonds in C is equal to $D(G_1) = D(G_2) = D(C) = 0$, namely, all the edges in C are M-single bonds. By the arbitrariness of M, all the edges in C are fixed single bonds. The same is true for the edges in a standard combination $\{C_1, C_2\}$ satisfying $D(C_1, C_2) = 0$.

Necessity: By the definition of an ED CS, G has a perfect matching, and hence conditions (1) and (2) hold (Theorem 2.6). We want to show that G has a SE-cut C of type I or a standard combination $\{C_1, C_2\}$ of type II consisting of fixed single bonds of G, and hence $D(C) = 0$, $D(C_1, C_2) = 0$.

By Lemma 3.3 G has at least one fixed single bond, say e, on C(o) or C(i) of G (see Fig. 9). By Lemma 3.2, G also has some non-fixed bonds. We distinguish two cases.

Case 1: e' is not a fixed double bond or e' does not belong to G (see Fig. 9). Then there is a perfect matching M of G such that e^* is an M-double bond. If e^{**} is an M-double bond too, then by Lemma 3.4 all the edges $e_1, \dots, e_n$ are fixed single bonds, where e_n is on C(o) or C(i) of G. Thus $C = \{e, e_1, \dots, e_n\}$ is a SE-cut consisting of fixed single bonds of G. If e^{**} is an M-single bond, then e_0'' is an M-double bond. We consider the following two subcases.

Subcase 1.1: e_o'' is a fixed double bond of G. If all the edges $e_1'', \dots, e_n''$ are fixed double bonds of G, then $C = \{e, e_1, \dots, e_n\}$ is a SE-cut consisting of fixed single bonds of G. Now suppose that $e_1'', \dots, e_t''$ $(t < n)$ are fixed double bonds of G, but e_{t+1}'' is not a fixed double bond. Then there is a perfect matching M' of G such that $\hat{e}$ is an M'-double bond. e_t'' is certainly an M'-double bond since it is a fixed double bond of G. Note that $\tilde{e}$ is a fixed single bond of G. By Lemma 3.4 all the edges $\tilde{e}_1, \dots, \tilde{e}_m$ are fixed single bonds of G. Hence $C' = \{e, e_1, \dots, e_t, \tilde{e}, \tilde{e}_1, \dots, \tilde{e}_m\}$ is a SE-cut consisting of fixed single bonds of G.

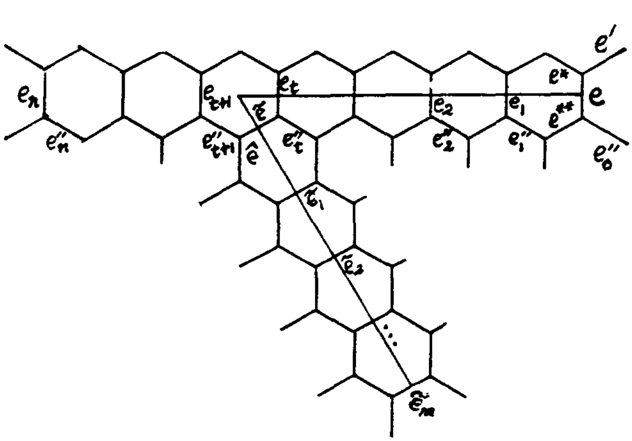

Fig. 9.

Subcase 1.2: e_0'' is not a fixed double bond. Then there exists a perfect matching $M^* \neq M$ such that e^{**} is an M^*-double bond. It is not difficult to see that the edges of $M \oplus M^*$ constitute several M-alternating cycles which are also M^*-alternating cycles. e_0'' and e^{**} belong to one of them, say P^*. We claim that e^* cannot be on P^*. Otherwise, an odd length cycle P^{**} consisting of a segment of P^* and the edge e is found, contradicting that G is bipartite and has no cycle with odd length. Now let $\bar{M} = M \oplus E(P^*)$. Both e^* and e^{**} are $\bar{M}$-double bonds. Hence $C = \{e, e_1, \dots, e_n\}$ is a SE-cut consisting of fixed single bonds of G as mentioned at the beginning of Case 1.

Case 2: e' is a fixed double bond of G. This case can be dealt with in a similar way as in Subcase 1.1. We omit the details.

We have shown that each fixed single bond of G on $C(\mathrm{o})$ or $C(\mathrm{i})$ determines a SE-cut consisting of fixed single bonds of G. If one of these determined SE-cuts, say C, is of type I, then both of the two components G_1 and G_2 of $G - C$ have perfect matchings. Thus $|B(G_i)| = |W(G_i)|$, for $i = 1, 2$. Therefore, $D(C) = D(G_1) = D(G_2) = 0$, and C is a SE-cut having the required property, and the theorem is proved. Now suppose that all the SE-cuts determined by fixed single bonds on $C(\mathrm{o})$ or $C(\mathrm{i})$ are of type II.

If G has only one fixed single bond e on $C(\mathrm{o})$, which determines a SE-cut C of type II, delete all the fixed single bonds in C and other fixed single bonds of G (if any), delete all fixed double bonds of G (if any) together with their end vertices. The resultant graph must be some disjoint HSs without fixed bonds. All the edges of $C(\mathrm{o}) - e$ must belong to one of these HSs since $C(\mathrm{o}) - e$ has no fixed bonds of G. Let the HS to which $C(\mathrm{o}) - e$ belongs be G^*. Evidently, all the edge of $C(\mathrm{o}) - e$ are on the perimeter of G^* and are contained in an M^*-alternating cycle for some perfect matching M^* of G^* (Lemma 3.5). There is no doubt that M^* can be extended to form a perfect matching M of G. Hence we can say that all the edges of $C(\mathrm{o}) - e$ are contained in an M-alternating cycle for some perfect matching M of G. Since e is a chord of this M-alternating cycle i.e. e has two end vertices on the M-alternating cycle, e is also on an M-alternating cycle, contradicting that e is a fixed single bond of G (Lemma 3.1). This contradiction indicates that G has more than one fixed single bond on $C(\mathrm{o})$.

Among the SE-cuts which are determined by the fixed single bonds on $C(\mathrm{o})$ and consist of fixed single bonds of G, if there are two, say C_1 and C_2, forming a standard combination, then both G_1 and G_2 of $G - \{C_1, C_2\}$ have perfect matchings. Hence we have $|B(G_i| = |W(G_i)|$ for $i = 1, 2$. Therefore, $D(C_1, C_2) = D(G_1) = D(G_2) = 0$. We now assume that any two SE-cuts of type II determined by fixed single bonds on $C(\mathrm{o})$ do not form a standard combination. We label the edges on $C(\mathrm{o})$ clockwise as $e_1, e_2, \dots, e_q$, where e is a fixed single bond of G. If two adjacent edges e_i and e_{i+1} are both fixed bonds ($1 \leqslant i \leqslant q$, $i+1$ is taken modulo q), then one is a fixed single bond and the other must be a fixed double bond. Since if both are fixed single bonds, the two SE-cuts determined by e_i and e_{i+1}, respectively, will form a standard combination, a contradiction. Let $e_1, \dots, e_f$ be alternately fixed single bonds and fixed double bonds of G. Since e_f must be a fixed single bond of G, $f \equiv 1 \pmod q$ or $f < q$. If $f \equiv 1 \pmod q$, $C(\mathrm{o})$ is an M-alternating cycle for every perfect matching M of G, contradicting that e_1 is a fixed single bond (Lemma 3.1). Hence $f < q$. Now let

$e_{f+1}, \ldots, e_{f+t}$ $(f + t \leqslant q)$ be non-fixed bonds of G, and e_{f+t+1} be a fixed single bond of G $(f + t + 1 \equiv 1 \pmod q$ or $f + t + 1 < q)$. By an analogous reasoning as above, $e_{f+1}, \ldots, e_{f+t}$ are on the perimeter of a HS H which is subgraph of $G - \{C_f, C_{f+t+1}\}$ and has no fixed bonds, where C_f and C_{f+t+1} are SE-cuts of type II determined by e_f and e_{f+t+1}, respectively. By Lemma 3.5 the perimeter of H is an M'-alternating cycle for some perfect matching M' of H. Since H is a subgraph of G by deleting fixed bonds, M' can be extended to form a perfect matching M of G. Because $\{C_f, C_{f+t+1}\}$ is not a standard combination by our assumption, t must be an odd positive integer. W.l.o.g., we may assume that $e_{f+1}, \ldots, e_{f+t}$ are alternately M-double bonds and M-single bonds with the first and the last (i.e. e_{f+1} and e_{f+t}) being M-double bonds. Now $e_1, \ldots, e_f, e_{f+1}, \ldots, e_{f+t}, e_{f+t+1}$ are alternately M-single bonds and M-double bonds for some perfect matching M of G. If $f + t = q$, then $C(\mathrm{o})$ of G is already an M-alternating cycle. If $f + t < q$, we can repeat the above discussion and finally come to the conclusion that $C(\mathrm{o})$ of G is an M-alternating cycle for some perfect matching M of G. Then the fixed single bond e_1 is contained in an M-alternating cycle of G, a contradiction. This contradiction implies that G must have a standard combination $\{C_1, C_2\}$, where C_1 and C_2 are two SE-cuts of type II consisting of fixed single bonds of G, and are determined by two fixed single bonds on $C(\mathrm{o})$. As reasoning above, $\{C_1, C_2\}$ satisfies $D(C_1, C_2) = 0$.

The proof is thus completed. $\square$

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